Antiferromagnetic fluctuations in the superconducting phase of low- and high-temperature superconductors

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Abstract

Based on recent experimental results for electron-doped cuprate oxides and ferromagnetic superconductors, it is shown that antiferromagnetic fluctuations always develop in the superconducting phase of both low- and high-temperature superconductors. The relation between the magnitude of the antiferromagnetic pseudogap and the characteristic temperature of the antiferromagnetic pseudogap opening is obtained. The characteristic temperature of the antiferromagnetic pseudogap opening for metal superconductors is estimated.

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Recently, it was shown by means of inelastic neutron diffraction measurements [1] that earlier discovered in electron-doped cuprate oxides $R_{2-x}Ce_xCuO_4$, where R= Sm, Nd, Pr, (in the angle resolved photoemission measurements) [2] the antiferromagnetic pseudogap Δ^* corresponds to antiferromagnetic fluctuations in the superconducting phase of this cuprate superconductors (for a review see Ref. 3). The magnitude Δ^* of the antiferromagnetic pseudogap is much larger than the magnitude Δ of the superconducting gap, and the characteristic temperature T^*_{AFM} of the antiferromagnetic pseudogap opening essentially exceeds the critical temperature T_c of the superconducting transition. Such a behavior is typical for high-temperature superconductors, if normally observed in them above T_c pseudogap Δ^* can be identified with the antiferromagnetic pseudogap corresponding to antiferromagnetic fluctuations with a finite lengthscale. Here we show that antiferromagnetic fluctuations develop in the superconducting phase of both low- and high-temperature superconductors and estimate the magnitude Δ^* of the antiferromagnetic pseudogap, the characteristic length scale l of antiferromagnetic fluctuations, and also, for metal superconductors, the characteristic temperature T^*_{AFM} of the antiferromagnetic pseudogap opening.

Recent detailed studies of the AC magnetic susceptibility $\chi(T)$ as a function of the temperature T in the ferromagnetic superconductor $ErRh_4B_4$ with the critical temperature $T_c = 8.7K$ and the Curie temperature $T_{FM} = 0.97K$ [4] have revealed a maximum of $\chi(T)$ at the temperature $T^*_{AFM} \cong 2K$ (in fields $H \cong 3kOe$), which can be interpreted as the manifestation of strong antiferromagnetic fluctuations in the superconducting phase of this low-temperature superconductor. This interpretation is supported by the sequence of phase transitions in the other ferromagnetic superconductor $ErNi_2B_2C$: the ferromagnetic transition with the transition temperature $T_{FM} = 2.3K$, the antiferromagnetic transition with the transition temperature $T_{AFM} = 6K$, and the superconducting transition with $T_c = 11K$.

Thus, we have similar sequences of transitions:

$ErRh_4B_4$	$T_{FM} = 0.97K$	$T^*_{AFM} \cong 2K$	$T_c = 8.7K$

$ErNi_2B_2C$	$T_{FM} = 2.3K$	$T_{AFM} = 6K$	$T_c = 11K$

These results suggest that antiferromagnetic fluctuations are present in the superconducting phase of conventional, low-temperature superconductors. (The above ferromagnetic superconductor $ErRh_4B_4$ is type I superconductor, as it is shown in Ref.4). However, the characteristic temperature T^*_{AFM} of the antiferromagnetic pseudogap opening is, in the case of low-temperature superconductors, less than the critical temperature T_c of the superconducting transition (contrary to the case of high-temperature cuprate superconductors).

Recently, it was shown [5] that the melting of a crystalline solid occurs when the critical number density n_c of vacancies is achieved, the critical number density of vacancies being

$$n_c \cong n_0 exp\left(-\alpha\right), \tag{1}$$

where $n_0 \approx 1.1 \times 10^{22} cm^{-3}$ and $\alpha \approx 18$ are quantum constants [6]. The length scale

$$d_c = n_c^{-1/3} \cong a_0 exp\left(\alpha/3\right) \cong 180nm, \tag{2}$$

where $a_0 = n_0^{-1/3} \cong 0.45nm$, can be interpreted as the size of a crystalline domain which cannot contain more than one vacancy. This interpretation is supported by the experimental results on the recryctallization of thin Al foils [7]. The recrystallization occurs only if the foil thickness d exceeds the length scale d_c, in more thin films there were no additional vacancies to nucleate the recrystallization [7].

This concept can be extended on other phase transitions, such as ferroelectric, ferromagnetic, and superconducting, if we consider the corresponding phase transition as the melting of some lattice. In the case of the ferroelectric transition, it is the lattice of electrical dipoles; in the case of the ferromagnetic transition, it is the lattice of magnetic dipoles. In the case of the superconducting phase transition, the situation is more complex, since the electron degrees of freedom are essentially involved. However, as it will be shown below, the above concept holds for superconducting transitions too.

The thermodynamic consideration based on the Clausius- Clapeyron equation gives the number density n_v of vacancies in a solid in the form [6]

$$n_v = (P_0/T)\, exp\,(-E_v/T) = (n_0 T_0/T)\, exp\,(-E_v/T)\,, \tag{3}$$

where E_v is the energy of the vacancy formation, $P_0 = n_0 T_0$ is a constant, T_0 can be put equal to the melting temperature of the solid at ambient pressure, and the Boltzmann constant k_B is included in the definition of the temperature T.

The energy of the vacancy formation E_v depends linearly on the pressure P (in the region of high pressures) as given by the formula

$$E_v = E_{v0} - \alpha P/n_0, \tag{4}$$

where α is a dimensionless constant, $\alpha \approx 18$ for sufficiently high pressures. On the atomic scale, the pressure dependence of the energy of the vacancy formation in the equation (4) is produced by the strong atomic relaxation in a crystalline solid under high pressure.

According to the equations (3) and (4), the number density of vacancies in a solid increases with increasing pressure (in the region of high pressures),

$$n_v = (n_0 T_0/T)\, exp\,(-\left(E_{v0} - \alpha P/n_0\right)/T)\,. \tag{5}$$

Consider now the number density n of elementary excitations in a corresponding lattice, instead of the number density of vacancies in an ordinary lattice. An elementary excitation invokes the change of the sign of the electrical or magnetic dipole moment of the elementary lattice cell for ferroelectrics and ferromagnets, respectively. In the case of superconductors, an elementary excitation is more complex.

Similarly to the energy of the vacancy formation (4), the energy E of an elementary excitation depends on the pressure (in the region of high pressures) as follows

$$E = E_0 - \alpha_P P/n_0, \tag{6}$$

where E_0 is the energy of an elementary excitation at ambient pressure, and α_P is a dimensionless constant dependent on the type of the phase transition. The pressure dependence of the energy of an elementary excitation in the equation (6) is produced by the atomic relaxation in the corresponding lattice under high pressure.

The pressure dependence of the number density n of elementary excitations is given by the formula analogous to the equation (5),

$$n = (n_0 T_c/T)\, exp\,(-\,(E_0 - \alpha_P P/n_0)\,/T)\,, \tag{7}$$

where T_c denotes here the transition temperature at ambient pressure.

The corresponding phase transition occurs when the critical number density n_c of elementary excitations (one elementary excitation per crystalline domain) is achieved. (Inelastic neutron diffraction measurements [1] have revealed that, on cooling, the antiferromagnetic phase transition occurs when the characteristic length l of antiferromagnetic fluctuations achieves the size of a crystalline domain given by the equation (2), $l \cong 400a_0$.) In view of the equation (7), it means that, on the phase equilibrium curve in the high pressure region, we have

$$(E_0 - \alpha_P P/n_0)\,/T \cong E_0/T_c \cong \alpha. \tag{8}$$

The equation (8) gives the pressure dependence of the transition temperature T in the region of high pressures in the form

$$T \cong T_c - (\alpha_P/\alpha)\, P/n_0. \tag{9}$$

The dimensionless slope of the phase equilibrium curve is given by the formula

$$k = n_0 dT/dP \cong -\alpha_P/\alpha. \tag{10}$$

Similarly to the case of the melting of crystalline solids, the relations (9) and (10) are valid only for sufficiently high pressures. In the region of relatively low pressures, the sign of dT/dP can be positive (the transition temperature may increase with pressure).

The superconducting phase diagram of Li metal [8] gives $k \approx -1/96$ and $\alpha_P \approx -k\alpha \approx 3/16$ for sufficiently high pressures, if we assume the relation $P' \approx 200P$ between the real pressure P and the measured pressure P'. (The problem of the calibration of high pressures is considered in Ref.6). These values of k and α_P are characteristic for low-temperature superconductors (see data for Al, Sn, Pb in Ref.9).

The superconducting phase diagram of the cuprate oxide $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$ [10] gives $k \approx -1/48$ and $\alpha_P \approx -k\alpha \approx 3/8$, for sufficiently high pressures. These values of k and α_P

are characteristic for high-temperature superconductors (see, for example, data for MgB_2 in Ref. 11 and data for Rb_3C_{60} in Ref. 9).

The values of k and α_P for ferroelectrics are $k \approx -1/9$ and $\alpha_P \approx -k\alpha \approx 2$ (see data for $BaTiO_3$ in Ref. 12). In the case of ferromagnets, $k \approx -2/9$ and $\alpha_P \approx -k\alpha \approx 4$ (see data for the weak itinerant ferromagnet $SrRuO_3$ in Ref. 13).

In accordance with the equation (8), the energy E_0 of an elementary excitation at ambient pressure is given by the relation

$$E_0 \cong \alpha T_c. \tag{11}$$

In the case of MgB_2 with $T_c = 39K$, the energy of an elementary excitation has an order of the Debye temperature θ_D: $E_0 \cong \alpha T_c \cong 700K$, whereas $\theta_D = 800 \pm 80K$ [14, 15, 16].

If we assume that at $T \cong 0$ the transition pressure P_c has an order of the melting pressure $P_m \cong n_0 T_m$, where T_m is the melting temperature of the solid at ambient pressure [6], then

$$\alpha_P \cong n_0 E_0/P_c \cong E_0/T_m \cong \theta_D/T_m, \tag{12}$$

for superconductors with $E_0 \cong \theta_D$. For most of metals, the ratio of the Debye temperature to the melting temperature is $\theta_D/T_m \cong 0.2 - 0.4$.

The magnitude $2\Delta^*$ of the antiferromagnetic pseudogap is equal to the energy E_0 of an elementary antiferromagnetic excitation, so that, in accordance with the equation (11), we have

$$2\Delta^* \cong \alpha T^*_{AFM} \quad , \tag{13}$$

where T^*_{AFM} is the characteristic temperature of the antiferromagnetic pseudogap opening. Optical measurements in $Nd_{2-x}Ce_xCuO_4$ and $Pr_{2-x}Ce_xCuO_4$ give the relation $2\Delta^*/T^*_{AFM} \approx 16$ [3], which is close to the relation (12), since $\alpha \approx 18$.

The experimental data suggest that the magnitude 2Δ of the superconducting gap is given by the relation

$$2\Delta \cong \alpha_P \alpha T_c. \tag{14}$$

For low-temperature superconductors $\alpha_P \approx -k\alpha \approx 3/16$ and the equation (14) gives

$$2\Delta \cong 3.4T_c. \tag{15}$$

This estimation of the magnitude of the superconducting gap is consistent with experimental data for Al, In, Sn obtained in the tunneling experiments [17]. Other experimental techniques give slightly different ratios of the magnitude of the superconducting gap to the critical temperature, maybe due to the interplay between the superconducting gap and the antiferromagnetic pseudogap (see below).

For high-temperature superconductors $\alpha_P \approx -k\alpha \approx 3/8$ and from the equation (14) we obtain

$$2\Delta \cong 7T_c. \tag{16}$$

The ratio $2\Delta/T_c$ measured in $Sm_{2-x}Ce_xCuO_4$ by means of local tunneling spectroscopy is varying from 4 to 7 due to the local change in cerium content and, whence, in the value of the critical temperature [1]. The maximum value of $2\Delta/T_c$, corresponding to the maximum value of the critical temperature (which was the case in optimally doped samples used in these measurements) is in agreement with the relation (16).

The characteristic length l of antiferromagnetic fluctuations in the superconducting phase [3] has an order of magnitude of the diameter $2r_0$ of the atomic relaxation region [5],

$$l \cong 2r_0 \cong 2\alpha a_0 \cong 16nm, \tag{17}$$

or, more exactly,

$$l \cong 4\beta\alpha r_0 \cong 25nm, \tag{18}$$

if $\beta \cong 0.8$ wich is the case for most of metals [3].

Inelastic neutron diffraction measurements give the characteristic length of antiferromagnetic fluctuations in the superconducting phase of $R_{2-x}Ce_xCuO_4$ at the level of $l \approx 20nm$ [1,3], which is in agreement with the estimations (17) and (18). It means that antiferromagnetic fluctuations are connected with the atomic displacement, the region of antiferromagnetic fluctuations having its center at the position of the "lattice defect" associated with an elementary antiferromagnetic excitation.

Neutron diffraction studies of the ferromagnetic superconductor $ErRh_4B_4$ have established the existence of a modulated structure in the superconducting regions at the length scale $\cong 10nm$ [4]. This structure can be interpreted as the antiferromagnetic modulation with a length scale having an order of the radius of the atomic relaxation region $r_0 \cong \alpha a_0 \cong 8nm$ [5]. The size of superconducting regions of the supercooled superconducting phase of this ferromagnetic superconductor, coexisting with ferromagnetic domains in the narrow temperature interval $T \approx 0.9 - 0.97K$, has an order of the size of crystalline domains given by the equation (2). On heating, a sharp transition from the ferromagnetic phase to the superconducting phase is observed at $T_{FM} = 0.97K$ [4]. The ratio T_c/T_{FM} for this ferromagnetic superconductor is $T_c/T_{FM} \cong \alpha/2 \cong 9$.

Since $T^*_{AFM} \cong 2K$ and $T_c = 8.7K$, from the relation (13) we obtain for $ErRh_4B_4$:

$$2\Delta^* \cong \alpha T^*_{AFM} \cong 36K, \tag{19}$$

whereas the magnitude of the superconducting gap, according to the relation (15), is

$$2\Delta \cong 3.4T_c \cong 30K, \tag{20}$$

so that $2\Delta^* \cong 2\Delta$. For the other ferromagnetic superconductor $ErNi_2B_2C$, the equations (13) and (15) give $2\Delta^* \cong 110K$ and $2\Delta \cong 37K$, respectively, so that $\Delta^*/\Delta \cong 3$.

Since $2\Delta^* \cong 2\Delta$ for $ErRh_4B_4$, the antiferromagnetic phase transition is suppressed, contrary to the case of $ErNi_2B_2C$, where $\Delta^*/\Delta \cong 3$. In the case of weak itinerant ferromagnets UGe_2 and $URhGe$ [2], the relation $2\Delta^* \cong 2\Delta$ is also presumably valid, so that the antiferromagnetic transition is suppressed and the superconducting transition occurs instead. The characteristic temperature of the antiferromagnetic pseudogap opening can be determined from the relations (13) and (14) as follows

$$T^*_{AFM} \cong 2\Delta^*/\alpha \cong 2\Delta/\alpha \cong \alpha_P T_c. \tag{21}$$

Thus we obtain for these superconducting ferromagnets

UGe_2	$T^*_{AFM} \cong 0.2K$	$T_c = 0.95K$ (under pressure)	$T_{FM} = 33K$

URhGe	$T^*_{AFM} \cong 0.05K$	$T_c = 0.27K$	$T_{FM} = 9.5K$

The ratio T_{FM}/T_c for these ferromagnetic superconductors is $T_{FM}/T_c \cong 2\alpha$.

Since the antiferromagnetic transition is not normally observed in metal superconductors, the same relations $2\Delta^* \cong 2\Delta$ and $T^*_{AFM} \cong \alpha_P T_c$ are valid in this case too.

The ^{17}O nuclear magnetic resonance spectra of overdoped samples of the hole-doped high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ with $T_c = 75 - 90K$ [18] show a minimum of the linewidth of the O(1) resonance (corresponding to the oxygen in the CuO_2 plane) at the temperature $T^*_{AFM} \cong \alpha_P T_c$, where $\alpha_P \approx 3/8$. This minimum of the O(1) resonance linewidth corresponds to antiferromagnetic fluctuations in the superconducting phase of this cuprate superconductor and indicates that the relation $2\Delta^* \cong 2\Delta$ is valid also for overdoped cuprate superconductors. In the case of near-optimally doped sample with $T_c = 90K$ the increase of the Knight shift above T_c is indicative of the relation $2\Delta^* > 2\Delta$ in the region of optimal doping.

To summerize, we show that antiferromagnetic fluctuations develop in the superconducting phase of both low- and high-temperature superconductors, we obtain the temperature and pressure dependence of the number density of elementary excitations for ferroelectrics, ferromagnets and superconductors. We obtain further the curve of phase equilibrium in the high pressure region for ferroelectric, ferromagnetic and superconducting phase transitions. We give also the estimations of the magnitudes of the antiferromagnetic pseudogap and the superconducting gap, and of the characteristic length scale of antiferromagnetic fluctuations in the superconducting phase. We show that for metal superconductors (and other nonmagnetic low-temperature superconductors) the magnitudes of the antiferromagnetic pseudogap and the superconducting gap are close each to other and give the estimation of the characteristic temperature of the antiferromagnetic pseudogap opening for these superconductors.

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[1] E.M.Motoyama, G.Yu, I.M.Vishik, O.P.Vajk, P.K.Mang, and M.Greven, Nature **445**,

186 (2007).

[2] N.P.Armitage, D.H.Lu, C.Kim et al., Phys. Rev. Lett. **87**, 147003 (2001).

[3] A.Zimmers, Y.Noat, T.Cren, W.Sacks, D.Roditchev, B.Liang, and R.L.Greene, E-print archives, arXiv: 0705.4217 (cond-mat. supr-con) (2007).

[4] R.Prozorov, M.D.Vannette, S.A.Law, S.L.Bud'ko, and P.C.Canfield, E-print archives, arXiv: 0707.0029 (cond-mat. str-el) (2007).

[5] F.V.Prigara, E-print archives, arXiv: 0704.0972 (cond-mat. stat-mech) (2007).

[6] F.V.Prigara, E-print archives, cond-mat/0701148 (2007).

[7] B.S.Bokstein, S.Z.Bokstein, and A.A.Zhukhovitsky, *Thermodynamics and Kinetics of Diffusion in Solids* (Metallurgiya Publishers, Moscow, 1974).

[8] S.Deemyad and J.S.Schilling, Phys. Rev. Lett. **91**, 167001 (2003).

[9] J.S.Schilling, in *Handbook of High Temperature Superconductivity: Theory and Experiment*, editor J.R.Schrieffer, associated editor J.S.Brooks (Springer Verlag, Hamburg, 2007).

[10] M.K.Crawford, R.L.Harlow, S.Deemyad et al., Phys. Rev. B **71**, 104513 (2005).

[11] S.Deemyad, T.Tomita, J.J.Hamlin et al., Physica C **385**, 105 (2003).

[12] G.S.Zhdanov, *Solid State Physics* (Moscow University Press, Moscow, 1961).

[13] J.J.Hamlin, S.Deemyad, J.S.Schilling et al., E-print archives, cond-mat/0609149 (2006).

[14] Z.F.Wei, G.C.Che, F.M.Wang, M.He, and X.L.Chen, Modern Physics Lett. B **15**, 1109 (2001).

[15] T.Ichitsubo, H.Ogi, S.Nishimura, T.Seto, M.Hirao, and H.Inui, Phys. Rev. B **66**, 052514 (2002).

[16] J.L.Luo, J.Zhang, ZJ.Chen et al., Chinese Physics Lett. **18**, 820 (2001).

[17] D.Saint-James, G.Sarma, and E.J.Thomas, *Type II Superconductivity* (Pergamon Press, Oxford, 1969).

[18] B.Chen, S.Mukhopadhyay, W.P.Halperin, P.Guptasarma, and D.G.Hinks, E-print archives, arXiv:0707.3171 (cond-mat.supr-con) (2007).

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